Supporting Information

Effect of Polymerisation by Microwave on the Physical Properties of Molecularly Imprinted Polymers (MIPs) Specific for Caffeine

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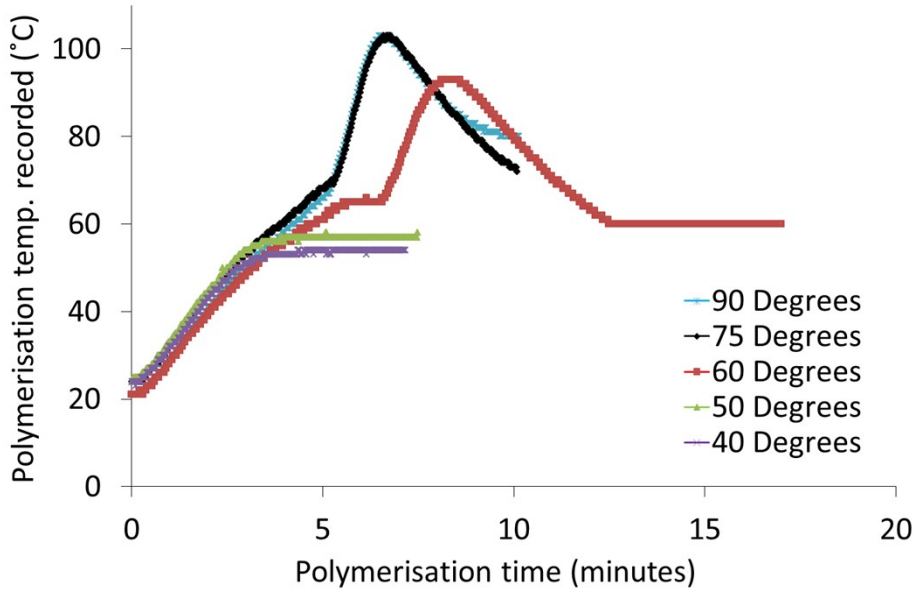
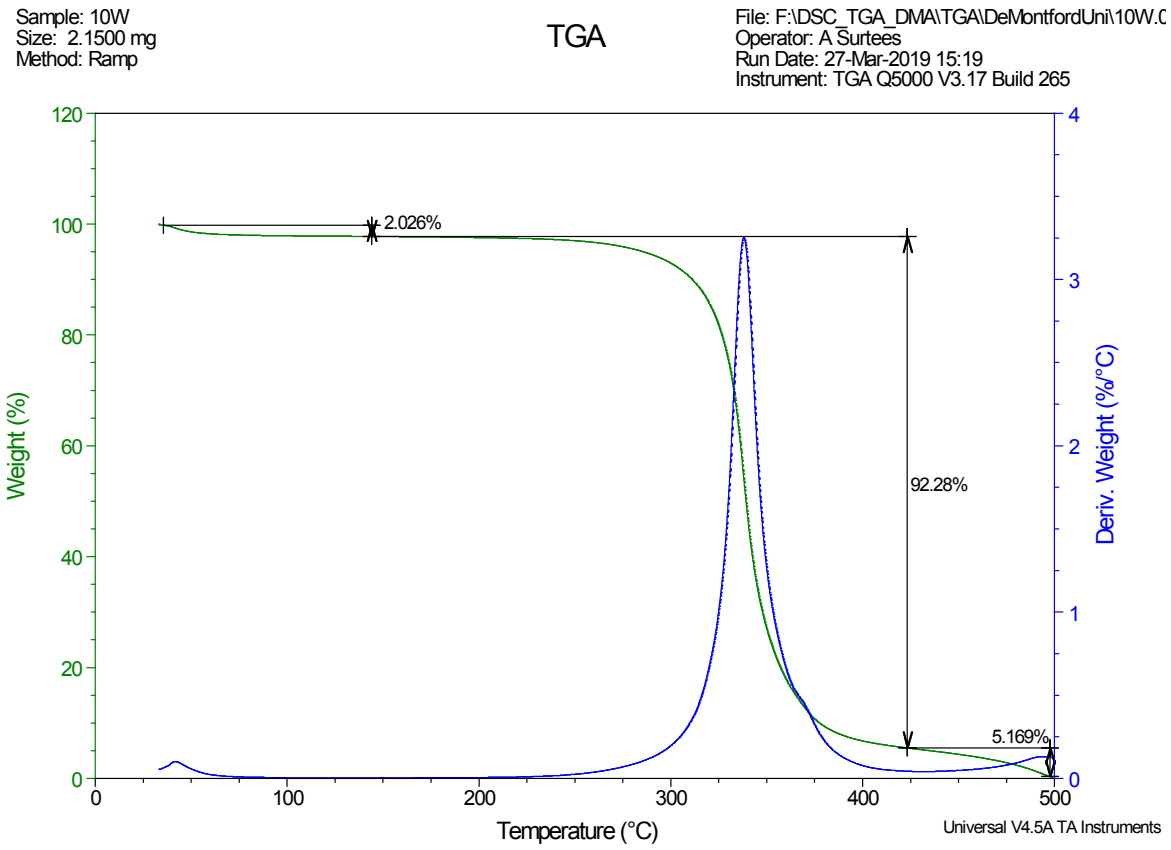


Supporting Information Figure 1: Varying Target Temperature with 5 W heating rate. This highlights that at least 60 °C (above AIBN decomposition temperature) is required at low power.

Thermal Analysis - Changes in Microwave Power

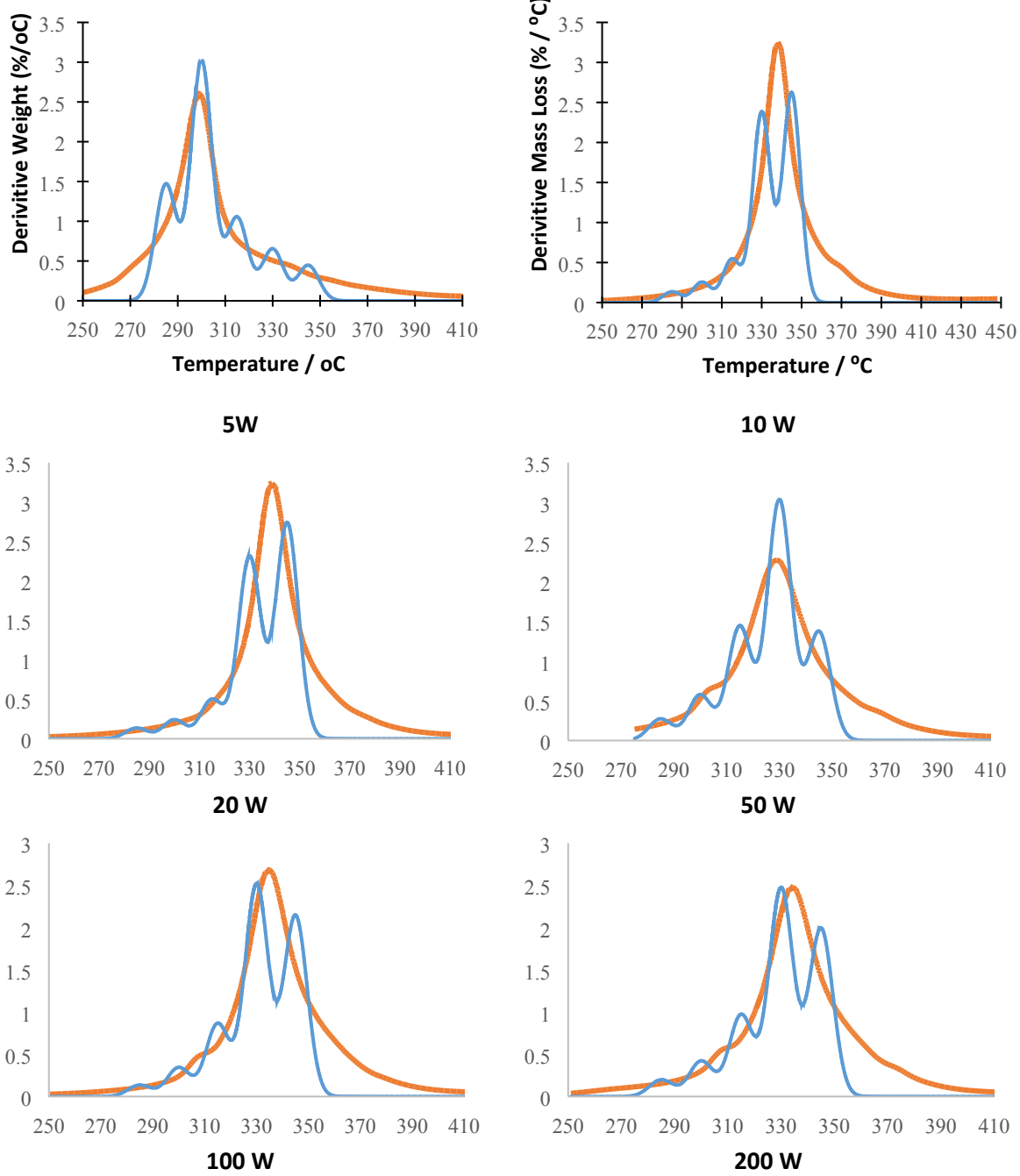


Supporting Information Figure 2: Example plot to show how the mass losses were compiled

Supporting Information Table 1: Trends from TGA Mass Loss Data

Sample	Mass loss 1 (%)	Mass loss 2 (%)	Mass loss 3 (%)
5W	2.889	90.53	6.381
10W	2.026	92.28	5.169
20W	2.113	92.22	5.052
50W	2.231	92.82	4.679
100W	2.092	91.81	5.404
200W	1.759	92.75	5.240

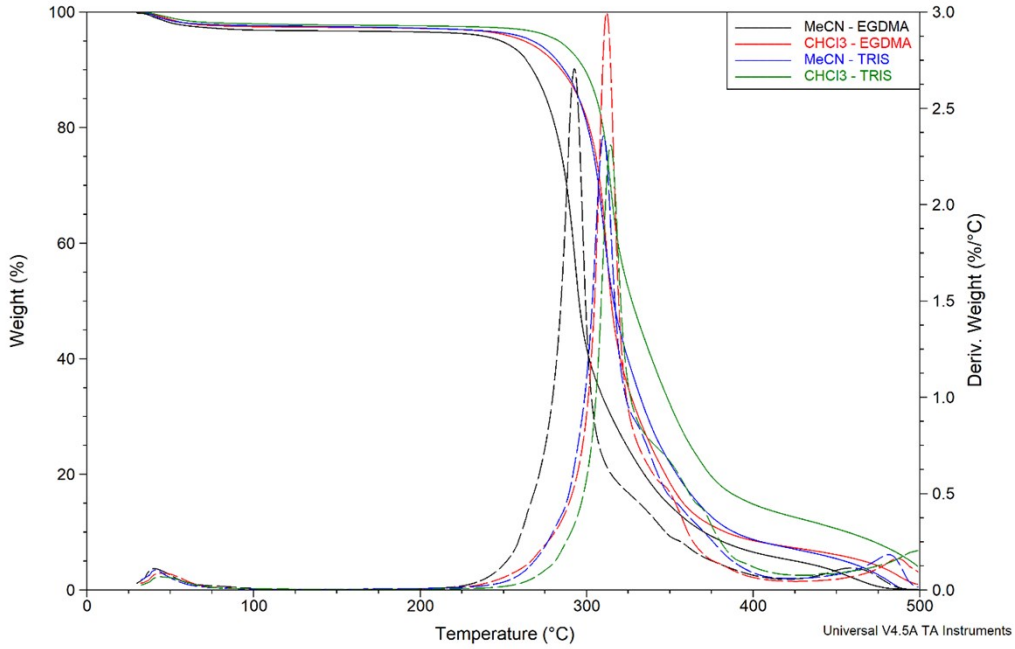
Thermal Analysis – TGA Peak Deconvolution



Supporting Information Figure 3: 5-peak deconvolution of derivative mass loss with temperature – raw data in orange, sum of the 5 deconvoluted peaks in blue.

Thermal Analysis - Changes in Solvent or Cross Linker

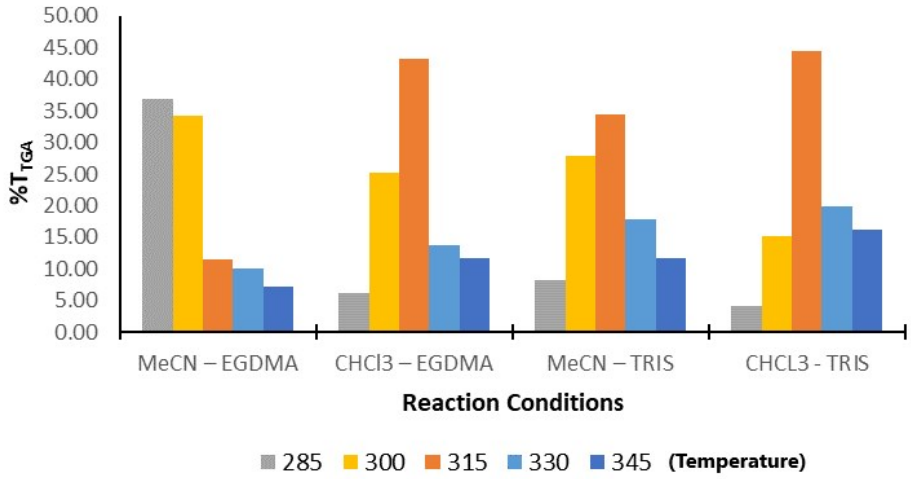
Samples recorded with varying solvent or crosslinker choices were analysed in a similar manner to the original samples. TGA decays of all four samples showed three degradation events.



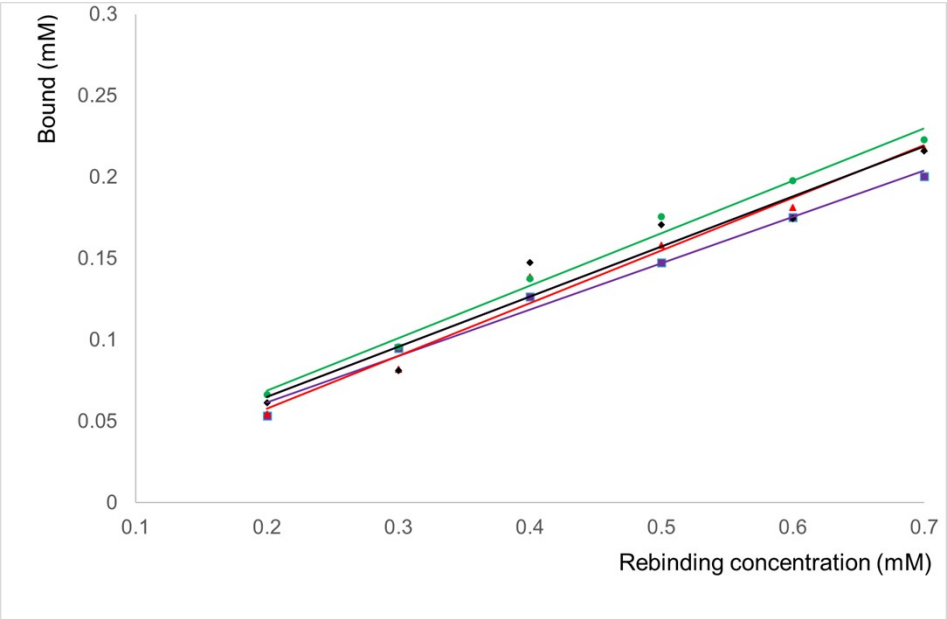
Supporting Information Figure 4: TGA curves with derivative mass losses of samples with varying solvent / cross linker

Supporting Information Table 2: Trends from TGA Mass Loss Data

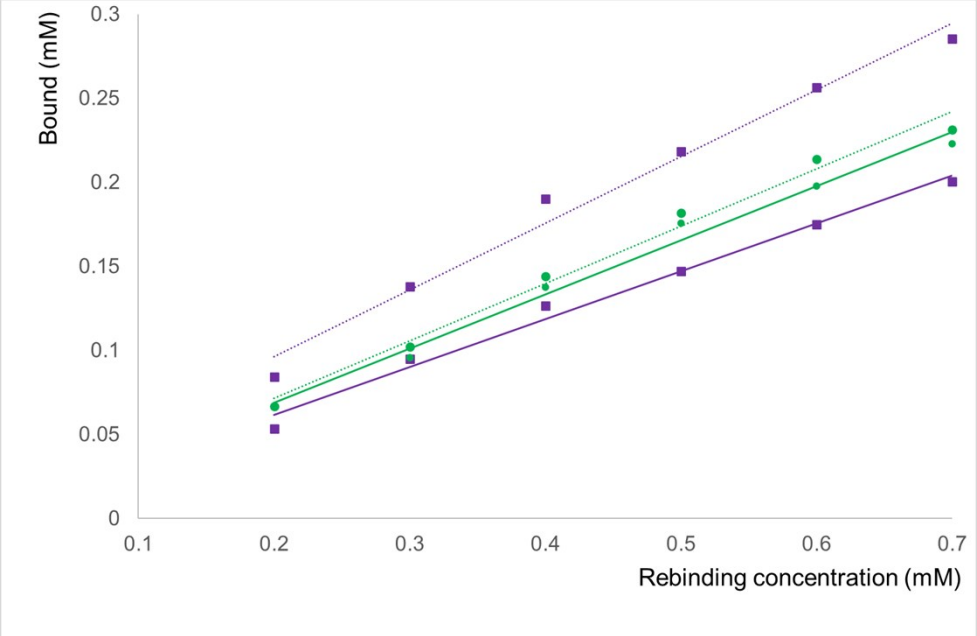
Sample	Tg (^{o}C)	Mass loss 1 (%)	Mass loss 2 (%)	Mass loss 3 (%)
MeCN – EGDMA	76.4	3.219	91.72	4.904%
$CHCl_3$ – EGDMA	79.2	2.657	90.07	6.319
MeCN – TRIS	77.4	2.585	90.44	7.186
$CHCL_3$ - TRIS	76.4	2.182	85.19	8.475



Supporting Information Figure 5: $\%T_{TGA}$ of derivative mass losses of samples with varying solvent / cross linker across 15 ^{0}C temperature ranges



Supporting Information Figure 6: Rebinding of caffeine at different concentrations for to NON-IMPRINTED polymers made at different powers. Purple square with purple line = 5 W. Red triangle with red line = 50 W. Black diamond with black line = 150 W. Green circle with green line = 300 W. Samples measured in triplicate. Standard deviations not shown for clarity.

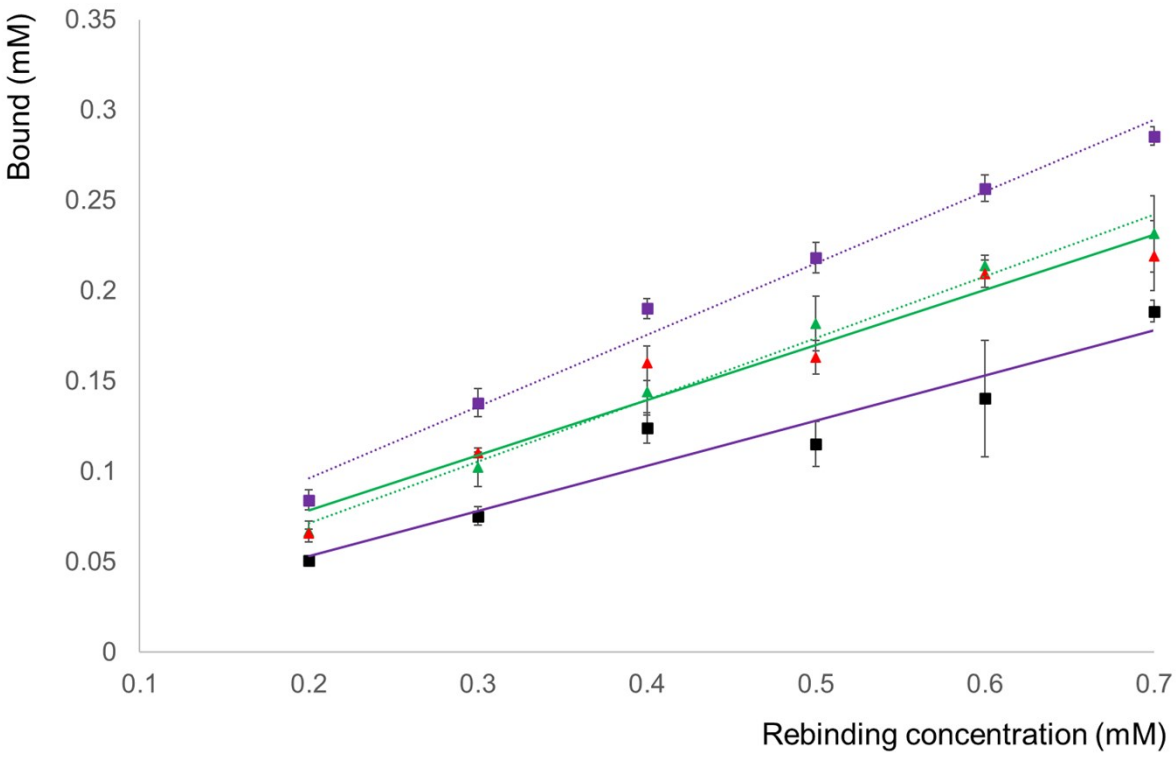


Supporting Information Figure 7: Rebinding of caffeine at different concentrations for to imprinted and non-imprinted polymers made at different powers. Samples measured in triplicate. Standard deviations not shown for clarity.
Purple square with purple dashed line = 5 W Imprinted.
Purple square with purple SOLID line = 5 W Non- imprinted.
Green circle with green dashed line = 300 W Imprinted.
Green circle with Green SOLID line = 300W Non-imprinted.

This highlights the differences between the highest studied power (300 W) and lowest (5 W). In both cases the imprints binds slightly more but the 5W exhibits less non-specific binding.

Supporting Table 3: Imprinting factors calculated for MIP at various rebinding concentrations.

Conc (mM)	5W	50W	150W	300 W
0.2	1.58	1.41	1.22	1.01
0.3	1.45	1.29	1.26	1.07
0.4	1.50	1.29	1.04	1.05
0.5	1.48	1.35	1.15	1.04
0.6	1.47	1.35	1.26	1.08
0.7	1.42	1.28	1.16	1.04
Average	**1.48**	**1.33**	**1.18**	**1.05**



Supporting Information Figure 8: Rebinding of caffeine and theophylline at different concentrations to imprinted polymers made at different powers. Samples measured in triplicate.
Purple square with purple dashed line = 5 W Caffeine rebinding
Black square with purple SOLID line = 5 W Theophylline rebinding
Green triangle with green dashed line = 300 W Caffeine rebinding
Red Triangle with Green SOLID line = 300W Theophylline rebinding

This figure demonstrates the lower power MIP (5 W) offers superior selectivity between caffeine and theophylline, compared to the higher power (300 W). Cross-binding is still relatively high due to the similar nature of theophylline to caffeine. Caffeine is a bulkier molecule (extra methyl) so cavity will be larger enabling smaller theophylline in.